

Supercurrents in an atom-molecule gas in an optical ring lattice

T. Wang,¹ J. Javanainen,¹ and S. F. Yelin^{1,2}

¹*Department of Physics, University of Connecticut, Storrs, CT 06269*

²*ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138*

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Atom and molecule currents in a Fermi gas in the neighborhood of a Feshbach resonance are studied in a one-dimensional optical ring lattice by directly diagonalizing small models. A rotational analogy of flux quantization is used to show that fraction of the current is carried by particles with twice the mass of an atom, which suggests pairing and superfluidity.

Artificial condensed-matter materials constructed by loading low-temperature atoms in an optical lattice hold promise as a means to explore major outstanding questions such as the origin of high- T_c superconductivity, to realize what heretofore have been fundamental thought experiments in condensed matter physics, and maybe to carry out quantum computations [1, 2]. The degree of control exerted by the experimenter in an optical lattice stands in stark contrast to condensed-matter systems supplied by Nature. For instance, the interactions between the atoms may be controlled by varying a magnetic field around a Feshbach resonance [3, 4, 5]. Photoassociation [6, 7, 8] could be similarly employed [9, 10].

In fact, though, Feshbach resonance and photoassociation entail conversion of atom pairs into molecules, and vice versa [11]. In this paper we study flows in an interconverting atom-molecule system in an optical lattice by direct numerical solutions of small systems. In a close analogy with past investigations of flux quantization [12], we analyze a one-dimensional optical lattice bent to a ring and rotated. We find indications for one facet of superfluidity with fermions, namely, that currents are carried by pairs of atoms reminiscent of Cooper pairs. Complete pairing may be approached at the Feshbach resonance when the atom-molecule coupling is strong, and when the magnetic field is varied across the resonance the carriers of the current smoothly change between atoms and molecules.

What constitutes superfluidity is an interesting question in its own right. In the experiments on superfluidity in optical lattices [13, 14] the criterion has been that, once released from the lattice, the atoms from different sites interfere. This, however, is an observation of off-diagonal long-range order, not necessarily of superfluidity. A persistent current is not a failsafe indicator of superfluidity either. In a mesoscopic ring that holds electrons and is threaded by a magnetic flux, the quantum mechanical ground state may carry a finite current. From this viewpoint, experimental observations of persistent currents in mesoscopic rings [15] are, perhaps, not surprising. Instead, a frequently used criterion for superfluidity in fermion systems is anomalous flux quantization. Basically, in phenomena associated with the presence of the magnetic field, the current appears to be carried by particles with twice the charge of an individual carrier [12, 16, 17].

Given that direct numerical solutions are feasible only in small systems, studies of long-range off-diagonal order that would model the experimental procedures [13, 14] are presently beyond our capabilities. We therefore look for anomalous flux quantization. The remaining problem with neutral atoms is that there is no direct coupling between magnetic field and the center-of-mass motion. In principle one could use laser-induced electromagnetic couplings to produce an effective gauge field on the atoms [18, 19, 20], but here we envisage using rotation of the atomic sample as a substitute for magnetic field.

Suppose that the prospective superfluid is tightly confined to a torus with the circumference L , and that in the direction of the torus, x , a rotated periodic potential $V(x - vt)$ is imposed, where v is the linear velocity along the torus. When one transforms the one-particle Schrödinger equations for the wave function $\psi(x, t)$ to a co-moving frame, $\xi = x - vt$, $\tau = t$, and defines $\psi(x, t) = e^{im(v^2\tau/2 + v\xi)/\hbar} \Psi(\xi, \tau)$, in the transformed Schrödinger equation the only remnant of the motion of the potential $V(x)$ is the twisting boundary condition $\Psi(\xi + L, \tau) = e^{-i\Phi} \Psi(\xi, \tau)$, where the rotation phase is $\Phi = mvL/\hbar$. The value of Φ only matters modulo 2π .

Next assume that the optical-lattice potential is deep enough to warrant a tight-binding approximation. The Wannier function for each site $k = 1, \dots, N_s$, may be introduced as usual, $u(x - x_k)$, but the annihilation operator of, say, a boson at site k , b_k , is chosen in such a way that the corresponding wave function is $e^{-ik\varphi} u(x - x_k)$, $\varphi = \Phi/N_s$ being the phase change from one lattice site to the next. The purpose of our convention is to revert the twisting boundary condition to the usual periodic boundary condition. The cost is altered phases of the hopping matrix elements, from a real t to $te^{\pm i\varphi}$, in the ensuing Hubbard type model.

The same approach works even if multiple interacting and interconverting species are present. We focus on a model in which two types of fermionic atoms (annihilation operators $c_{k\uparrow}$ and $c_{k\downarrow}$) may combine on-site to a diatomic bosonic molecule (b_k). The Hamiltonian becomes

$$\begin{aligned} \frac{H}{\hbar} = & -t_A \sum_{k, \sigma=\uparrow, \downarrow} (e^{i\varphi_A} c_{k+1, \sigma}^\dagger c_{k, \sigma} + \text{h.c.}) \\ & -t_M \sum_k (e^{i\varphi_M} b_{k+1}^\dagger b_k + \text{h.c.}). \end{aligned}$$

$$+ \delta \sum_k b_k^\dagger b_k + g \sum_k (b_k^\dagger c_{k\downarrow} c_{k\uparrow} + \text{h.c.}). \quad (1)$$

Here g is the coupling strength for atom-molecule conversion and δ is the detuning from the Feshbach resonance controlled by the magnetic field [21]. We have thereby formulated what is known as a two-channel theory, with atoms and molecules as separate albeit coupled degrees of freedom [11]. We take the masses of the \uparrow and \downarrow atoms to be equal, whereupon the mass of the molecules is twice the mass of the atoms and the two hopping phases satisfy $\varphi_M = 2\varphi_A$. Different-mass atoms lead to incommensurate situations that do not have magnetic-field counterparts, but we do not go there in this paper. Note that Hamiltonian (1) is the same as that for a ring lattice threaded by a magnetic field $B = 2m\varphi c/qL$ [22].

In the present model the conserved particle number $\hat{N} = \sum_k \hat{N}_k$ is a sum over the lattice sites of the local particle numbers $\hat{N}_k = c_{k\uparrow}^\dagger c_{k\uparrow} + c_{k\downarrow}^\dagger c_{k\downarrow} + 2b_k^\dagger b_k$. \hat{N}_k thus is a locally conserved quantity whose value only changes as a result of transport. This gives the identification of the operator for the current from the site k to the site $k+1$ as

$$\begin{aligned} \hat{I}_{k \rightarrow k+1} = & \sum_{\sigma=\uparrow,\downarrow} it_A (e^{i\varphi_A} c_{k+1,\sigma}^\dagger c_{k,\sigma} - e^{-i\varphi_A} c_{k,\sigma}^\dagger c_{k+1,\sigma}) \\ & + 2it_M (e^{i\varphi_M} b_{k+1}^\dagger b_k - e^{-i\varphi_M} b_k^\dagger b_{k+1}). \end{aligned} \quad (2)$$

If the system is in an energy eigenstate in which there is a steady flow of atoms and/or molecules along the lattice, the value of the current $I \equiv \langle \hat{I}_{k \rightarrow k+1} \rangle$ and the energy of the state $E(\Phi_A, \Phi_M)$ regarded as a function of the phase parameters satisfies

$$I = -\frac{1}{\hbar} \left(\frac{\partial E}{\partial \Phi_A} + 2 \frac{\partial E}{\partial \Phi_M} \right). \quad (3)$$

Since E is a period function of Φ with period 2π , so does I as shown by Eq. (3) [23]. Here we may also compute the current numerically from Eq. (2) and easily separate it to atomic and molecular components, but Eq. (3) is convenient for qualitative discussions.

A way to compare the results for different system sizes is needed in order to ascertain that the outcome is not determined by limitations of the numerics. To this end we first note that for a nonrotating lattice, $v = 0$ and $\varphi_{A,M} = 0$, the ground state is obviously translationally invariant and possesses a left-right symmetry: $\langle c_{k+1,\uparrow}^\dagger c_{k\uparrow} \rangle = \langle c_{k'+1,\uparrow}^\dagger c_{k'\uparrow} \rangle$ and $\langle c_{k+1,\uparrow}^\dagger c_{k\uparrow} \rangle = \langle c_{k-1,\uparrow}^\dagger c_{k\uparrow} \rangle$ for all k and k' . The expectation values $\langle c_{k+1,\uparrow}^\dagger c_{k\uparrow} \rangle$ are therefore real at $v = 0$. The motion of the lattice enters only through the phase parameters $\varphi_{A,M}$. Assuming that perturbation theory in $\varphi_{A,M}$ is valid, Eq. (2) shows that in the limit $v \simeq 0$ or $\varphi_{A,M} \simeq 0$ the current is a linear function of $\varphi_{A,M} = \Phi_{A,M}/N_s$. On the other hand, a sensible thermodynamic limit should be taken so that the number of lattice sites N_s and the invariant particle number N both tend to infinity in such a way that the average

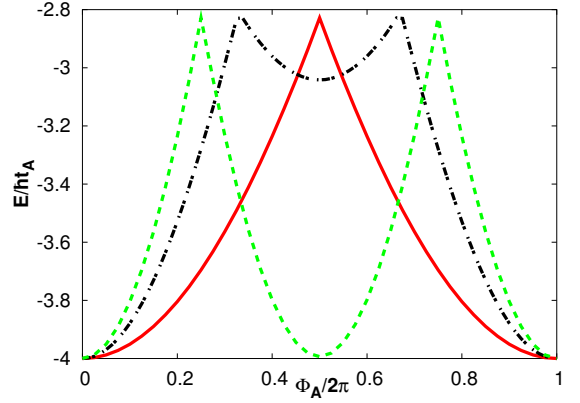


FIG. 1: (Color online) Ground state energy E as a function of the rotation phase Φ_A for $g = 0$ (solid line), $g/t_A = 5$ (dash-dotted line), and $g/t_A = 100$ (dashed line). The energies corresponding to $g/t_A = 5$ and $g/t_A = 100$ have been scaled linearly so that the ranges of E coincide for all three g . The fixed parameters are $\delta = 0$, $N_s = 4$, $N = 2$.

occupation number per site N/N_s remains a constant. Ground-state expectation values such as $\langle c_{k+1,\uparrow}^\dagger c_{k\uparrow} \rangle$ may be viewed as some functions $h_{\uparrow\uparrow}(N_s, N/N_s)$, and in the limit $N_s \rightarrow \infty$ with $N/N_s = \text{constant}$ they evidently tend to constants that depend only on the fixed ratio N/N_s . Putting these considerations together, we see that, for given total phases Φ_A and Φ_M , the only possible v -independent scaling of the current that leads to a nonzero and finite current in the thermodynamic limit is $I_T = N_s I$.

In this paper direct diagonalization based on the Lanczos algorithm [24] is employed to find the eigenvalue (energy) and eigenvector of the ground state of the Hamiltonian (1), and the results are then used to calculate various observables at zero temperature. In this approach arbitrary parameter values may be accommodated without approximations, although only for small numbers of atoms and lattice sites. From now on we use the value of the atomic tunneling matrix element t_A as the frequency scale. The number of \uparrow and \downarrow fermions is always the same. Until further notice we also assume that the molecules do not tunnel, whereupon $t_M = 0$ and the parameters φ_M and Φ_M do not enter at all.

We first study the resonance, $\delta = 0$, varying the coupling strength g . The dependence of $E(\Phi_A)$ on the phase Φ_A is the weaker the larger is the coupling g . The current I therefore decreases with g . With this in mind, we plot in Fig. 1 the energies E as a function of Φ_A for the coupling strengths $g/t_A = 0, 5$, and 100 , scaling the energy linearly in such a way that the minima and the maxima for each g coincide. The invariant particle number is $N = 2$, and the number of lattice sites is $N_s = 4$.

The main observation is that with increasing g the energy changes from being a 2π periodic function of Φ_A to having the period π . The current, basically the derivative $dE/d\Phi_A$, behaves as if it were a sum of two components

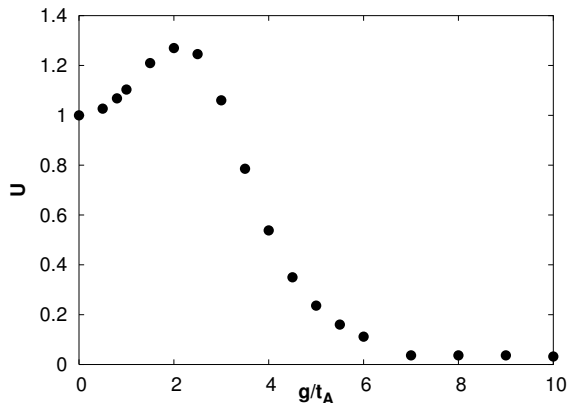


FIG. 2: (Color online) Unpaired fraction $U(g)$, a measure of the fraction of the current that is due to non-paired fermions, as a function of the coupling strength g . The fixed parameters are $\delta = 0$, $N_s = 8$, $N = 2$.

corresponding to the carrier masses m and $2m$, with the mass $2m$ taking over as the coupling strength is increased. In analogy with the earlier studies of the influence of the magnetic flux [12, 16, 17], we interpret this to mean that some of the fermions are paired, suggesting superfluidity. Moreover, the fraction of fermions appearing as pairs increases with increasing coupling strength.

We next quantify the fraction of the current that is due to unpaired fermions. One might think that Fourier analysis of $E(\Phi_A)$ gives straightforward answers, but there are problems. For instance, even with $g = 0$ and no pairing at all, there is still a Fourier component in $E(\Phi_A)$ with the period π . We therefore use the ratio of the Fourier component of the current with the period 2π to an estimate of the current, normalized so that the value at $g = 0$ equals unity, as the measure of the unpaired fraction. Specifically, we first find

$$f(g) = \frac{|\int_0^{2\pi} d\Phi \sin \Phi I(\Phi; g)|}{\max_{\Phi}[I(\Phi; g)] - \min_{\Phi}[I(\Phi; g)]}, \quad (4)$$

and define $U(g) = f(g)/f(0)$. A representative unpaired fraction U is plotted in Fig. 2 as a function of the coupling strength g , for $\delta = 0$, $N = 2$, $N_s = 8$. Unpaired fractions larger than unity are an unfortunate artifact of our definition, but the qualitative result is clear: With an increasing coupling strength the fraction of unpaired current carriers tends to zero.

To investigate the effects of the necessarily small size of the system on the results we draw in Fig. 3 the current scaled by the number of lattice sites, $I_T(\Phi_A) = N_s I(\Phi_A)$, as a function of the rotation phase Φ_A for the system sizes $N_s = 4$ and $N_s = 8$, both with $N/N_s = 1/2$. We set $\delta = 0$, and choose $g/t_A = 100$. If I_T were an invariant in the thermodynamic limit, in the limit of large N_s such curves should overlap. They do so quite well already in these small systems. Our interpretation is that, suitably scaled, the results for $N_s = 8$ and $N = 4$ already rep-

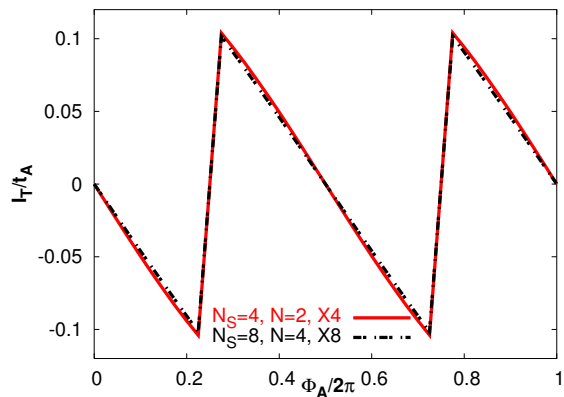


FIG. 3: (Color online) Scaled current as a function of the rotation phase for lattices with $N_s = 4$, $N = 2$ (solid line) and $N_s = 8$, $N = 4$ (dash-dotted line). The actual currents have been multiplied by the factors indicated in the legend. This figure is for Feshbach resonance, $\delta = 0$, and the atom-molecule coupling $g/t_A = 100$ ensures that the fermions are almost completely paired.

resent well the physics of the limit of a large number of lattice sites.

We have also looked into the effect of varying the atom number N for a fixed number of sites N_s on the fermion pairing behavior. In our numerics there is not much room for variation in N , and in a small system even a single unpaired fermion may make a major difference. With these caveats, in the strong-coupling case $g \gg t_A$ we have not detected a qualitatively significant effect of atom number on the fraction of paired fermions as long as the number of fermions is even.

In our final example we turn to the variation of the current with the detuning δ , the situation of BEC-BCS crossover where the system at near-zero temperature equilibrium is expected to change from an ideal Fermi gas to a BCS superfluid and then to a BEC of the diatomic molecules when the detuning is scanned across the resonance starting from a large positive value. In such a process the increasing fraction of molecules, the “bare” molecules denoted by b_k in our theory, has been observed experimentally [25] in a nonlattice gas, and successful comparisons of two-channel mean-field theories with the experiments have been reported [26, 27, 28]. Our model automatically leads to the period π for the molecular currents and as such says nothing about the superfluidity of the molecules, so that molecular currents are somewhat off the theme of the paper. Nonetheless, we shall demonstrate the change in the nature of the current carriers from atoms to molecules in a lattice upon the crossover.

In order to allow for molecular currents in the first place we need to choose a nonzero hopping matrix element t_M , thus we set $t_M = t_A$, and pick $g/t_A = 4.2$ so that about half of the current is expected to be paired according to Fig. 2. We plot in Fig. 4 both the total current and the atomic and molecular currents separately as

a function of the varying detuning δ . The system size is $N_s = 8$, $N = 4$. The expected smooth transition between atomic and molecular currents is observed.

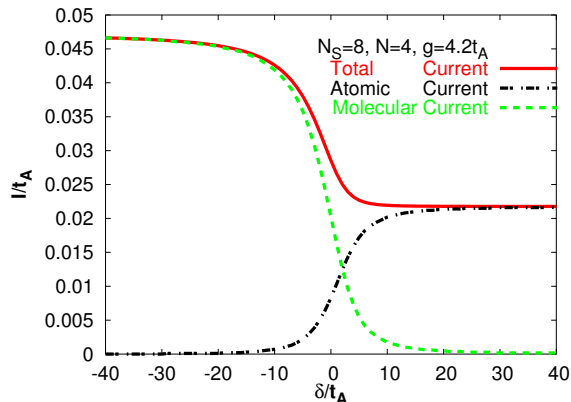


FIG. 4: (Color online) Total current (solid line), atomic current (dash-dotted line) and molecular current (dashed line) as a function of detuning in a lattice with $N_s = 8$, $N = 4$, $t_M/t_A = 1$, and $g/t_A = 4.2$.

Although our study is meant to be an in-principle theoretical discussion, a few comments about experiments are in order. Toroidal traps have been realized already [29], and there is a proposal to make an optical ring lattice [20]. As usual, the lattice potential results from interference between two light beams. Also as usual, the lattice potential may be made to move simply by taking the two beams to have different frequencies, here possibly by means of an optical delay line incorporating a (slowly) moving mirror. Analysis of the velocity distribution of the atoms has been discussed in Ref. [20]. Next, the coupling strength for the usual 834 G Feshbach resonance in

^6Li is large compared to the widths of the energy bands in any conceivable optical lattice. This implies that a single-band model such as (1) is inadequate [30]. A faithful realization of the Hamiltonian (1) may have to await further developments in photoassociation [31], which in principle permits a full control of the coupling strength. As the tunneling matrix elements are exponentially small in the mass of the particle, the case with $t_A \gg t_M$ is probably the experimental default. However, tunneling matrix elements can in principle be controlled with light by using optical transitions [32]. Overall, numerous and severe challenges must be overcome before our schemes are amenable to experiments, but the obstacles seem to be a matter of technology.

In sum, we have studied currents in an interconverting atom-molecule gas in an optical ring lattice by direct numerical solutions of small two-channel models. The center-of-mass motion of a neutral atom or molecule does not directly couple to the magnetic field, so we envisage rotation of the ring as a substitute to magnetic field for realizing an analog of flux quantization in a superconductor. We find flux quantization as if part of the current were carried by atom pairs, which constitutes indirect evidence for superfluidity. With an increasing atom-molecule coupling, an increasing fraction of the current is carried by atoms pairs. In analogy with the BEC-BCS crossover, variation of the magnetic field in the neighborhood of the Feshbach resonance leads to a smooth switching of the current carriers from atoms to molecules. The experimental challenges with our schemes are severe, but appear to be purely technical.

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